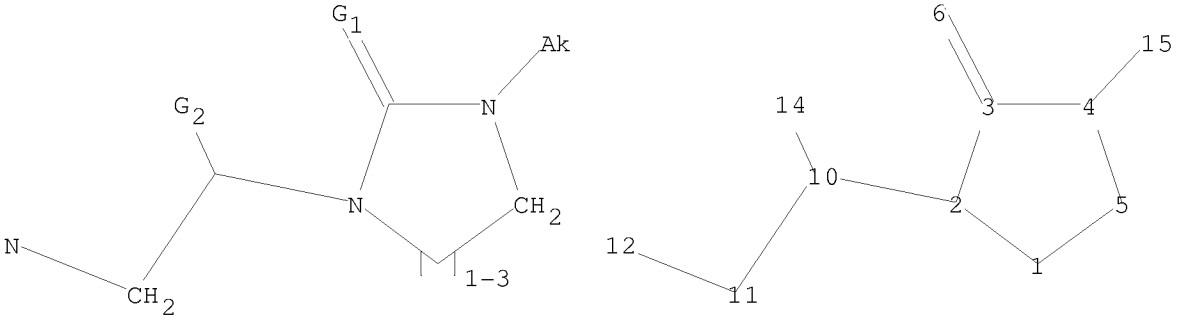
Uploading C:\Users\jcoppins\Documents\10593941.str



chain nodes :
6 10 11 12 14 15
ring nodes :
1 2 3 4 5
chain bonds :
2-10 3-6 4-15 10-11 10-14 11-12
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-15 10-14
exact bonds :
10-11 11-12

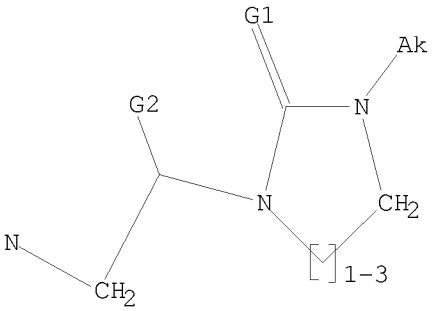
G1:O,S,N

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 10:CLASS 11:CLASS 12:CLASS
14:CLASS
15:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1:O,S,N

G2:H,Ak

Structure attributes must be viewed using STN Express query preparation.

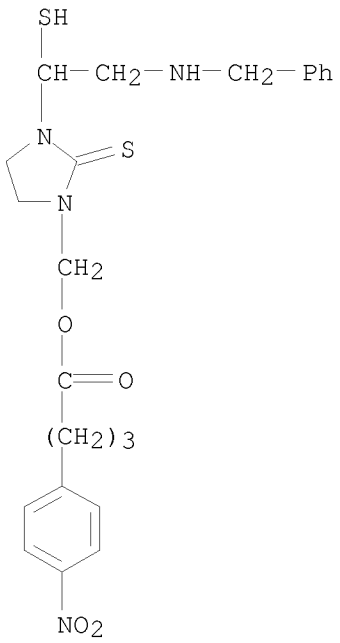
=> s l1 ful
FULL SEARCH INITIATED 20:26:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 240363 TO ITERATE

100.0% PROCESSED 240363 ITERATIONS 215 ANSWERS
SEARCH TIME: 00.00.03

L2 215 SEA SSS FUL L1

=> d l2 1-10

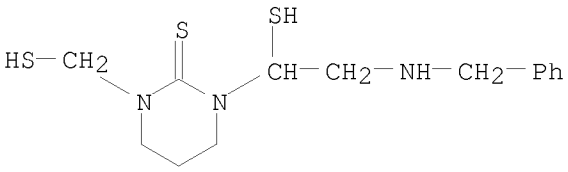
L2 ANSWER 1 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1349551-98-9 REGISTRY
ED Entered STN: 06 Dec 2011
CN Benzenebutanoic acid, 4-nitro-, [3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA INDEX NAME)
MF C23 H28 N4 O4 S2
SR Other Sources
Database: GVK BIO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

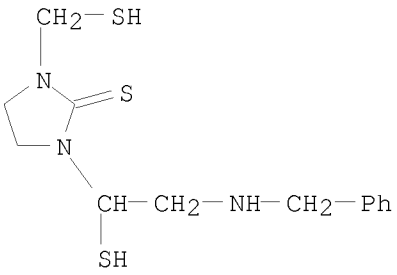
L2 ANSWER 2 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348962-28-6 REGISTRY
ED Entered STN: 05 Dec 2011

CN 2(1H)-Pyrimidinethione, tetrahydro-1-(mercaptomethyl)-3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]- (CA INDEX NAME)
MF C14 H21 N3 S3
SR Other Sources
Database: GVK BIO



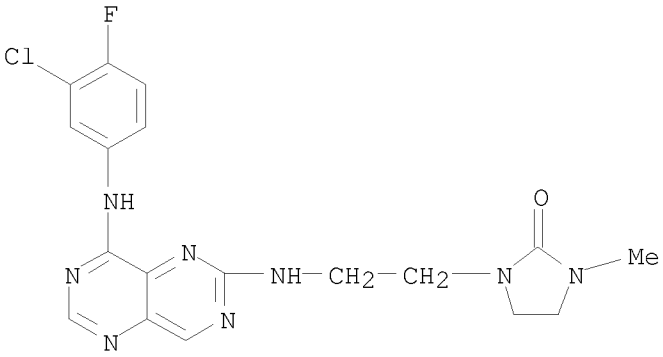
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 3 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348828-94-3 REGISTRY
ED Entered STN: 05 Dec 2011
CN 2-Imidazolidinethione, 1-(mercaptomethyl)-3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]- (CA INDEX NAME)
MF C13 H19 N3 S3
SR Other Sources
Database: GVK BIO



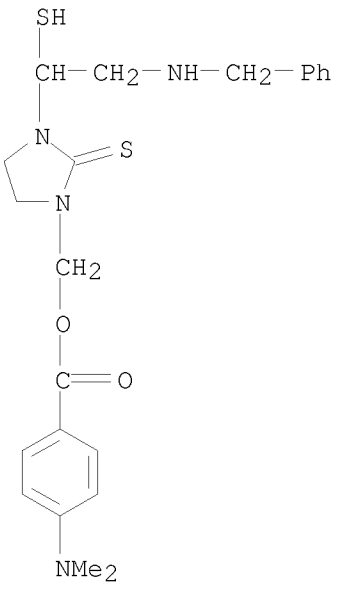
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 4 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348799-25-6 REGISTRY
ED Entered STN: 05 Dec 2011
CN 2-Imidazolidinone, 1-[2-[[8-[(3-chloro-4-fluorophenyl)amino]pyrimido[5,4-d]pyrimidin-2-yl]amino]ethyl]-3-methyl- (CA INDEX NAME)
MF C18 H18 Cl F N8 O
SR Other Sources
Database: GVK BIO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

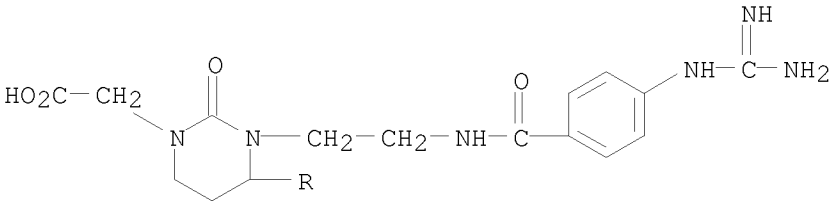
L2 ANSWER 5 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348516-48-2 REGISTRY
ED Entered STN: 04 Dec 2011
CN Benzoic acid, 4-(dimethylamino)-, [3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA INDEX NAME)
MF C22 H28 N4 O2 S2
SR Other Sources
Database: GVK BIO

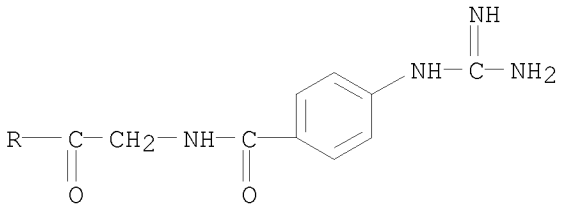


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 6 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN

RN 1348070-78-9 REGISTRY
ED Entered STN: 04 Dec 2011
CN 1(2H)-Pyrimidineacetic acid, 4-[2-[[4-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]-3-[2-[[4-[(aminoiminomethyl)amino]benzoyl]amino]ethyl]tetrahydro-2-oxo- (CA INDEX NAME)
MF C26 H32 N10 O6
SR Other Sources
Database: GVK BIO

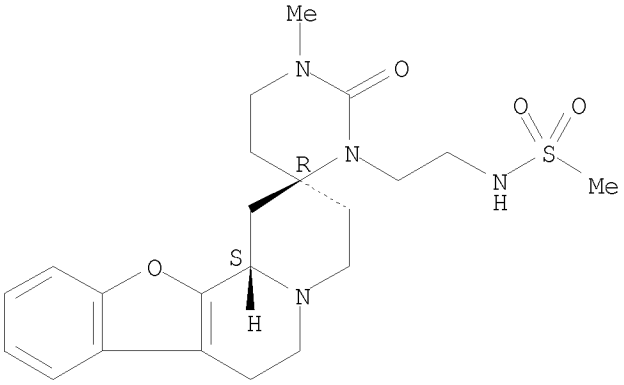




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

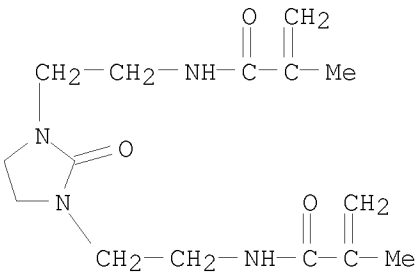
L2 ANSWER 7 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1347405-85-9 REGISTRY
ED Entered STN: 02 Dec 2011
CN INDEX NAME NOT YET ASSIGNED
FS STEREOSEARCH
MF C22 H30 N4 O4 S
SR Other Sources
Database: GVK BIO

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

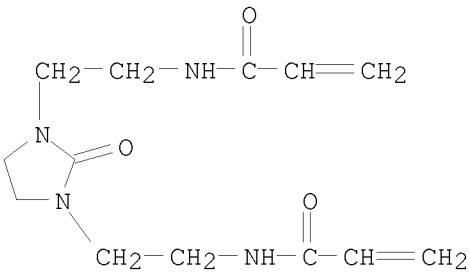
L2 ANSWER 8 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1346551-34-5 REGISTRY
ED Entered STN: 29 Nov 2011
CN INDEX NAME NOT YET ASSIGNED
MF C15 H24 N4 O3
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 9 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1346551-32-3 REGISTRY
ED Entered STN: 29 Nov 2011
CN INDEX NAME NOT YET ASSIGNED
MF C13 H20 N4 O3
SR CA
LC STN Files: CA, CAPLUS

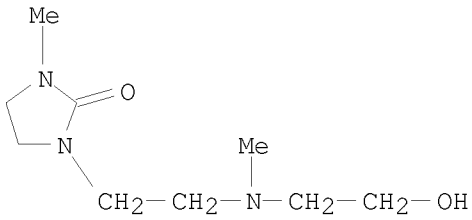


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 10 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1315512-37-8 REGISTRY
ED Entered STN: 09 Aug 2011
CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA INDEX NAME)
MF C9 H19 N3 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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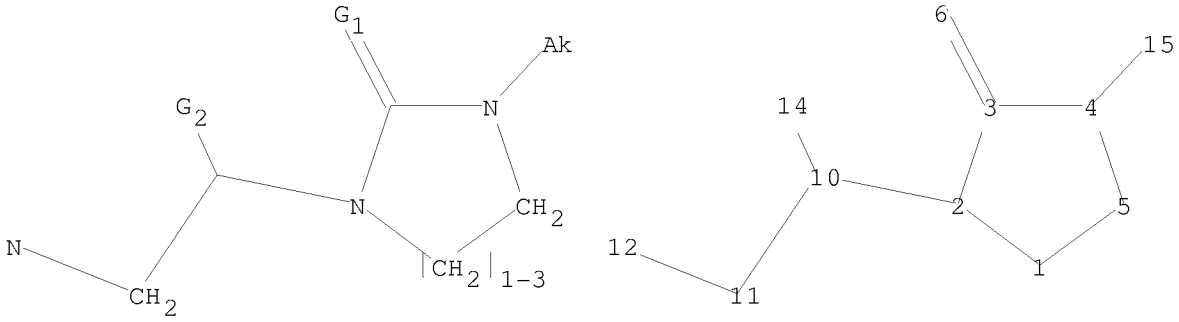
Uploading C:\Users\jcoppins\Documents\10593941a.str



chain nodes :
6 10 11 12 14 15
ring nodes :
1 2 3 4 5
chain bonds :
2-10 3-6 4-15 10-11 10-14 11-12
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-15 10-14
exact bonds :
10-11 11-12

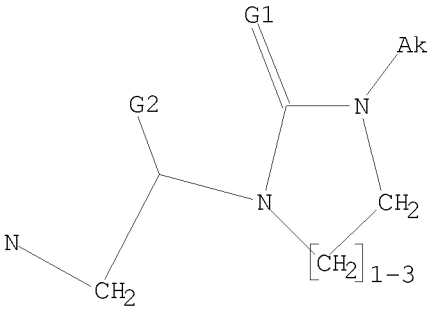
G1:O,S,N

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 10:CLASS 11:CLASS 12:CLASS
14:CLASS
15:CLASS

L3   STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3   STR



G1:O,S,N

G2:H,Ak

Structure attributes must be viewed using STN Express query preparation.

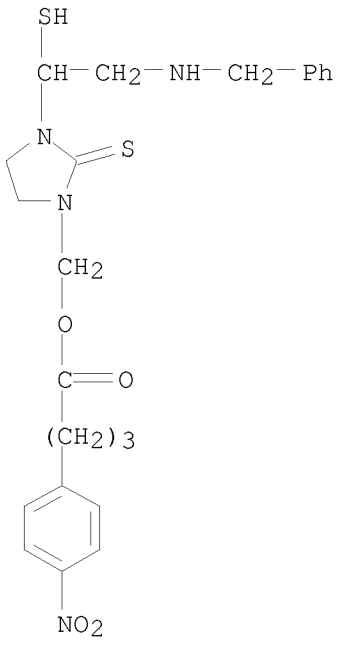
=> s l3 ful
FULL SEARCH INITIATED 20:30:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   240363 TO ITERATE

100.0% PROCESSED   240363 ITERATIONS   175 ANSWERS
SEARCH TIME: 00.00.04

L4   175 SEA SSS FUL L3

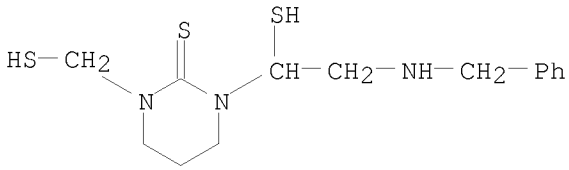
=> d l4 1-10

L4   ANSWER 1 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN   1349551-98-9 REGISTRY
ED   Entered STN: 06 Dec 2011
CN   Benzenebutanoic acid, 4-nitro-, [3-[1-mercapto-2-
     [(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA
     INDEX NAME)
MF   C23 H28 N4 O4 S2
SR   Other Sources
       Database: GVK BIO



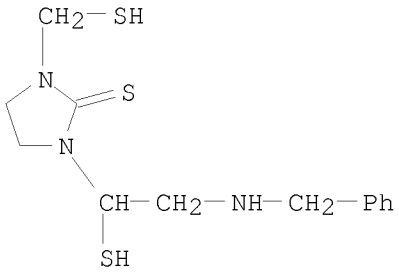
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 2 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348962-28-6 REGISTRY
ED Entered STN: 05 Dec 2011
CN 2(1H)-Pyrimidinethione, tetrahydro-1-(mercaptomethyl)-3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]- (CA INDEX NAME)
MF C14 H21 N3 S3
SR Other Sources
Database: GVK BIO



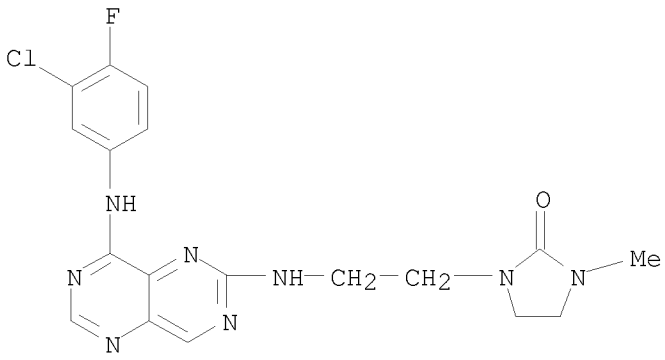
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 3 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348828-94-3 REGISTRY
ED Entered STN: 05 Dec 2011
CN 2-Imidazolidinethione, 1-(mercaptomethyl)-3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]- (CA INDEX NAME)
MF C13 H19 N3 S3
SR Other Sources
Database: GVK BIO



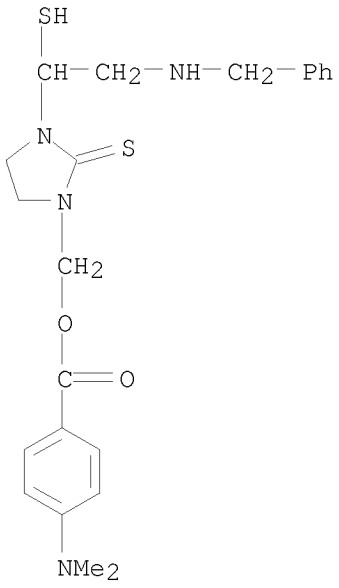
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 4 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348799-25-6 REGISTRY
ED Entered STN: 05 Dec 2011
CN 2-Imidazolidinone, 1-[2-[[8-[(3-chloro-4-fluorophenyl)amino]pyrimido[5,4-d]pyrimidin-2-yl]amino]ethyl]-3-methyl- (CA INDEX NAME)
MF C18 H18 Cl F N8 O
SR Other Sources
Database: GVK BIO



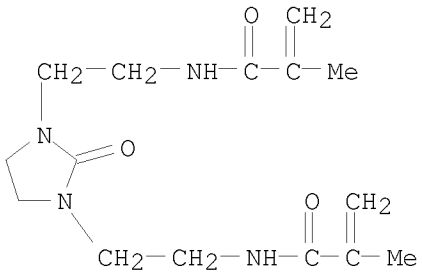
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 5 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1348516-48-2 REGISTRY
ED Entered STN: 04 Dec 2011
CN Benzoic acid, 4-(dimethylamino)-, [3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA INDEX NAME)
MF C22 H28 N4 O2 S2
SR Other Sources
Database: GVK BIO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 6 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1346551-34-5 REGISTRY
ED Entered STN: 29 Nov 2011
CN INDEX NAME NOT YET ASSIGNED
MF C15 H24 N4 O3
SR CA
LC STN Files: CA, CAPLUS

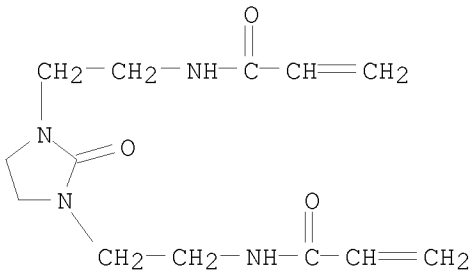


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 7 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1346551-32-3 REGISTRY
ED Entered STN: 29 Nov 2011
CN INDEX NAME NOT YET ASSIGNED
MF C13 H20 N4 O3

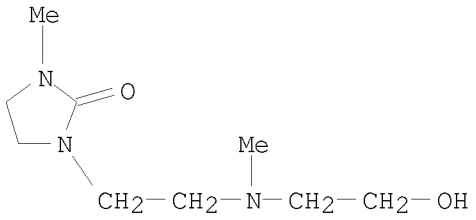
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 8 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1315512-37-8 REGISTRY
ED Entered STN: 09 Aug 2011
CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA INDEX NAME)
MF C9 H19 N3 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

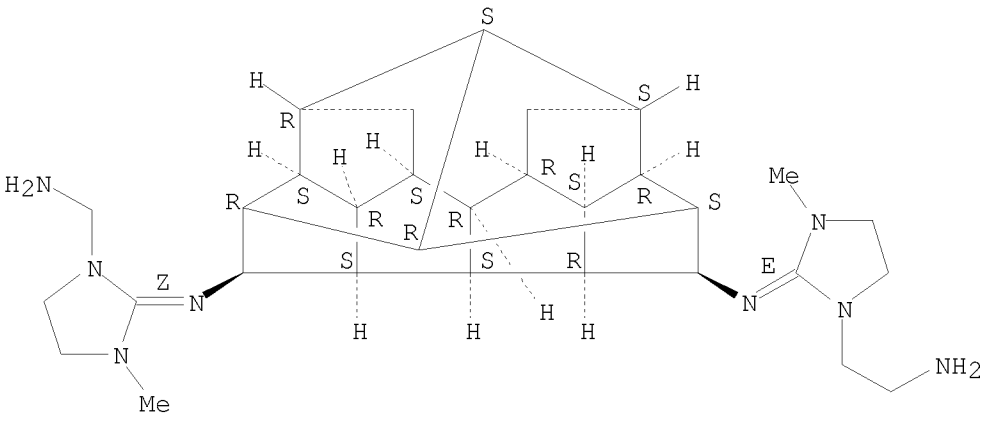


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 9 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1261062-12-7 REGISTRY
ED Entered STN: 28 Jan 2011
CN 2,7,3,6-Ethanediylidenedipentaleno[1,6-ab:1',6'-ef]pentalene-1,8-diamine, N1-[1-(2-aminoethyl)-3-methyl-2-imidazolinylidene]-N8-[1-(aminomethyl)-3-methyl-2-imidazolinylidene]octadecahydro-, stereoisomer (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H46 N8
SR CA
LC STN Files: CA, CAPLUS

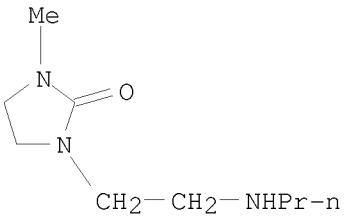
Relative stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 10 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1250017-79-8 REGISTRY
ED Entered STN: 01 Nov 2010
CN 2-Imidazolidinone, 1-methyl-3-[2-(propylamino)ethyl]- (CA INDEX NAME)
MF C9 H19 N3 O
SR Chemical Catalog
Supplier: Ukrorgsyntez Ltd.
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	440.80	441.03

FILE 'CAPLUS' ENTERED AT 20:31:42 ON 14 DEC 2011
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

FILE COVERS 1907 - 14 Dec 2011 VOL 155 ISS 25
FILE LAST UPDATED: 13 Dec 2011 (20111213/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2011
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2011

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2011.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> s l4
L5          61 L4

=> d l5 1-10 ibib abs hitstr
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L5 ANSWER 1 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2011:1427380 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 155:639066
TITLE: Semi-acrylic polyurethane aqueous coating compositions with good adhesion and scratch and chemical resistance
INVENTOR(S): Choi, Myeong Gi; Yang, Ji Won; Lim, Myeong Hyeok; Lee, Deok Hui
PATENT ASSIGNEE(S): KCC Corp., S. Korea
SOURCE: Repub. Korean Kongkae Taeho Kongbo, 7pp.
CODEN: KRXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Korean
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2011120610	A	20111104	KR 2010-40091	20100429

PRIORITY APPLN. INFO.: KR 2010-40091 20100429

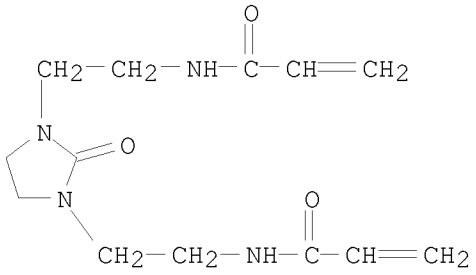
AB Title compns. contain a chlorinated polyolefin, an acrylic polyolefin, a film-forming resin, a water-dispersible polyurethane, and a crosslinking agent.

IT 1346551-32-3DP, polymers with polyolefin acrylate
RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(blend with chlorinated polyolefin and polyurethane; semi-acrylic

polyurethane aqueous coating compns. with good adhesion and scratch and chemical resistance)

RN 1346551-32-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



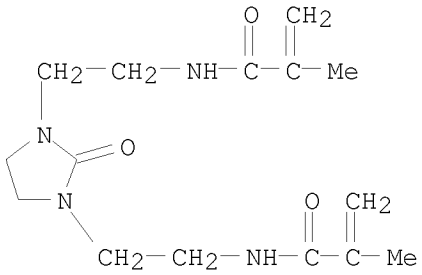
IT 1346551-34-5DP, polymers with polyolefin acrylate

RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(semi-acrylic polyurethane aqueous coating compns. with good adhesion and scratch and chemical resistance)

RN 1346551-34-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L5 ANSWER 2 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2011:740834 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 155:250356

TITLE: Degradation of MMEA at absorber and stripper conditions

AUTHOR(S): Lepaumier, Helene; Grimstvedt, Andreas; Vernstad, Kai; Zahlsen, Kolbjorn; Svendsen, Hallvard F.

CORPORATE SOURCE: Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, N-7491, Norway

SOURCE: Chemical Engineering Science (2011), 66(15), 3491-3498 CODEN: CESCAC; ISSN: 0009-2509

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

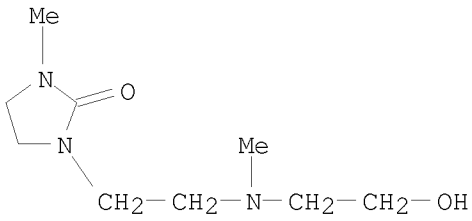
AB This study examines the degradation of N-methylethanolamine (MMEA) under different exptl. conditions. Thermal degradation with and without CO2, and oxidative degradation are studied. Samples of the degraded solution were taken

at regular intervals and analyzed. The percentage of amine loss was determined by liquid chromatog.-mass spectrometry (LC-MS) while the degradation compds. were identified and quantified by gas chromatog.-mass spectrometry (GC-MS). MMEA degradation at absorber and stripper conditions is compared with previous work on 2-ethanolamine (MEA). Degradation mechanisms are proposed and discussed in order to understand the differences compared to MEA.

IT 1315512-37-8
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(degradation of methylethanolamine at absorber and stripper conditions)

RN 1315512-37-8 CAPLUS

CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2011:20015 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 154:132821

TITLE: Preparation of sulfonylaminobutanamide derivatives for use as HIV protease inhibitors

INVENTOR(S): Flentge, Charles A.; Chen, Hui-Ju; Degoey, David A.; Flosi, William J.; Grampovnik, David J.; Huang, Peggy P.; Kempf, Dale J.; Klein, Larry L.; Krueger, Allan C.; Madigan, Darold L.; Randolph, John T.; Sun, Minghua; Yeung, Ming C.; Zhao, Chen

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S. Pat. Appl. Publ., 230pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

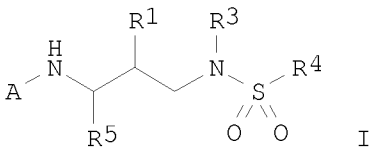
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20110003827	A1	20110106	US 2004-9841		20041210
PRIORITY APPLN. INFO.:			US 2003-529121P	P	20031211

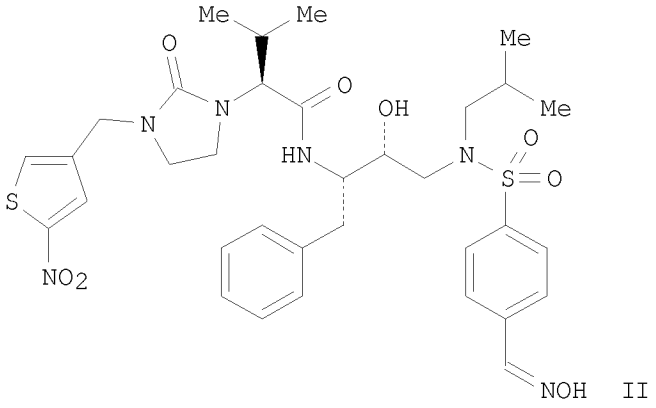
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 154:132821

GI



I



II

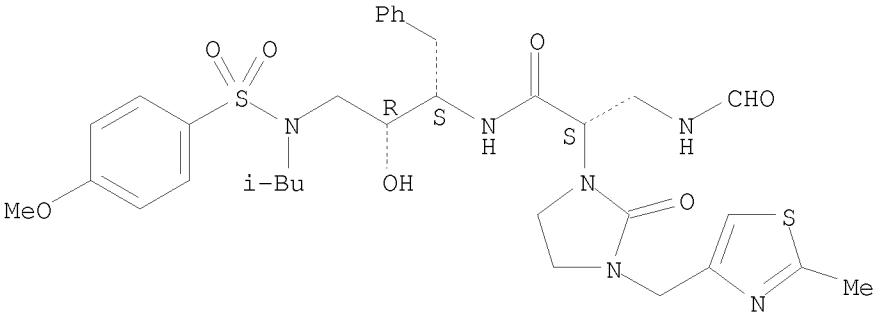
AB Title compds. I [A = C(O)alkyl, (un)substituted SO2-aryl, SO2-heteroaryl, etc.; R1 = OH, OSO2H, OPO3H, etc.; R3 = (un)substituted cycloalkyl, aryl, heteroaryl, etc.; R4 = (un)substituted cycloalkyl, cycloalkenyl, heterocyclyl, aryl, or heteroaryl; R5 = (un)substituted alkyl, alkenyl, cycloalkyl, arylalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as HIV protease inhibitors. Thus, e.g., II was prepared by a multistep procedure (preparation given). I were evaluated for activity against wild-type HIV or the passaged variants and demonstrated EC50 values in the range of 1 nM to 100 nM.

IT 854742-89-5P 854742-90-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonylaminobutanamide derivs. for use as HIV protease inhibitors)

RN 854742-89-5 CAPLUS

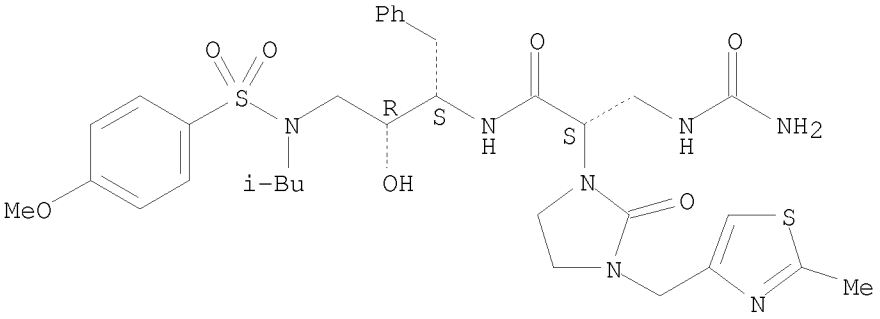
CN 1-Imidazolidineacetamide, α-[(formylamino)methyl]-N-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



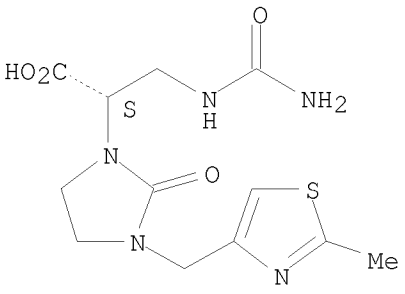
RN 854742-90-8 CAPLUS
CN 1-Imidazolidineacetamide, α-[[(aminocarbonyl)amino]methyl]-N-[(1S,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-, (αS)-
(CA INDEX NAME)

Absolute stereochemistry.



IT 1056133-73-3P 1056133-74-4P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonylaminobutanamide derivs. for use as HIV protease inhibitors)
RN 1056133-73-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

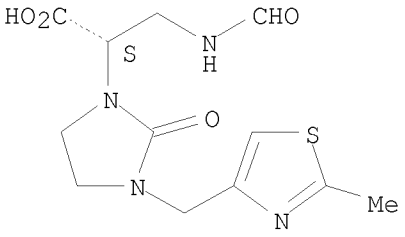
Absolute stereochemistry.



RN 1056133-74-4 CAPLUS
CN 1-Imidazolidineacetic acid, α-[(formylamino)methyl]-3-[(2-methyl-4-

thiazolyl)methyl]-2-oxo-, (αS)- (CA INDEX NAME)

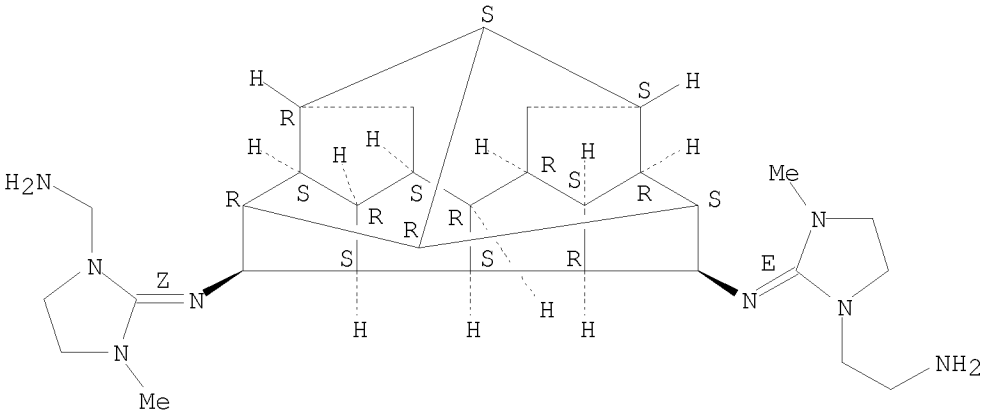
Absolute stereochemistry.



L5 ANSWER 4 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2010:1447837 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 154:132766
TITLE: Exceptional Superbasicity of Bis(guanidine) Proton Sponges Imposed by the Bis(secododecahedrane) Molecular Scaffold: a Computational Study
AUTHOR(S): Margetic, Davor; Ishikawa, Tsutomu; Kumamoto, Takuya
CORPORATE SOURCE: Laboratory for Physical-Organic Chemistry, Division of Organic Chemistry and Biochemistry, Ruder Boskovic Institute, Zagreb, 10001, Croatia
SOURCE: European Journal of Organic Chemistry (2010), (34), 6563-6572, S6563/1-S6563/106
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The exceptional superbasicity of a series of bis(guanidines) with a bis(secododecahedrane) mol. scaffold was found in the course of a computational study. The 3-syn,13-syn-disubstituted bis(secododecahedrane) skeleton ensures that nitrogen lone pairs of electrons are in close proximity, and the rigid framework of the polycyclic cage guarantees acid/base properties similar to those of proton sponges. Amine functionalization with alkyl substituents, imines, and guanidines leads to high basicity. Based on DFT computations, bis(guanidine)-bis(secododecahedrane) proton sponges with a (1,3-dimethylimidazolidin-2-ylidene)amino moiety are predicted to have very high basicities, both in the gas phase and acetonitrile. This skeleton provides the highest proton affinity (PA) value among all the aliphatic proton sponges reported (288.7 kcal mol-1, whereas the gas-phase basicity is 284.3 kcal mol-1, at the B3LYP/6-311+G**//B3LYP/6-31G* level). In acetonitrile the calculated PA is 319.4 kcal mol-1 and the estimated pKa is 38.5. Substitution of bis(secododecahedrane) with the intrinsically more basic nitrogen functionalities increases the PA to 316.3 kcal mol-1 and the pKa to 46.
IT 1261062-12-7
RL: PRP (Properties)
(exceptional superbasicity of bis(guanidine) proton sponges imposed by the bis(secododecahedrane) Mol. scaffold)
RN 1261062-12-7 CAPLUS
CN 2,7,3,6-Ethanediylidenedipentaleno[1,6-ab:1',6'-ef]pentalene-1,8-diamine, N1-[1-(2-aminoethyl)-3-methyl-2-imidazolinylidene]-N8-[1-(aminomethyl)-3-methyl-2-imidazolinylidene]octadecahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:1554838 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 152:262611
TITLE: Synthesis and Evaluation of Novel Compounds as Potent Dipeptidyl Peptidase IV Inhibitors
AUTHOR(S): Wang, Liutang; Zhang, Bin; Ji, Jianxin; Li, Bogang; Yan, Jufang; Zhang, Weiyu; Wu, Yong; Wang, Xuechao; Hou, Hui
CORPORATE SOURCE: West China School of Pharmacy, Sichuan University, Chengdu, 610041, Peop. Rep. China
SOURCE: Synthetic Communications (2010), 40(1), 52-57
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 152:262611
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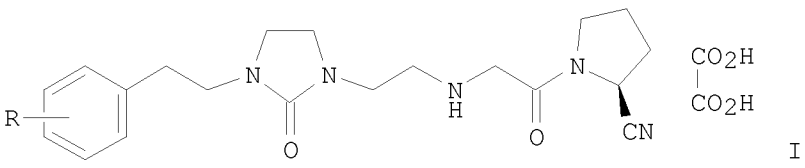


I

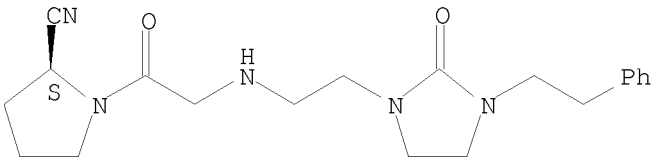
AB A series of new 2-cyanopyrrolidine derivs. I [R = H, 4-F, 3-MeO, etc.] with constrained imidazolidin ring were synthesized, Their structures were confirmed by 1H NMR spectroscopy and/or mass spectrometry, and their activities were evaluated in vitro. They were proven to possess submicromolar inhibitory activities against dipeptidyl peptidase IV.
IT 1145965-96-3P 1207841-08-4P 1207841-10-8P
1207841-12-0P 1207841-14-2P 1207841-16-4P

1207841-18-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and evaluation of cyanopyrrolidine derivs. as dipeptidyl peptidase IV inhibitors)
RN 1145965-96-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[2-oxo-3-(2-phenylethyl)-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

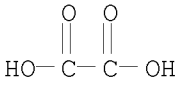
CRN 1145965-78-1
CMF C20 H27 N5 O2

Absolute stereochemistry.

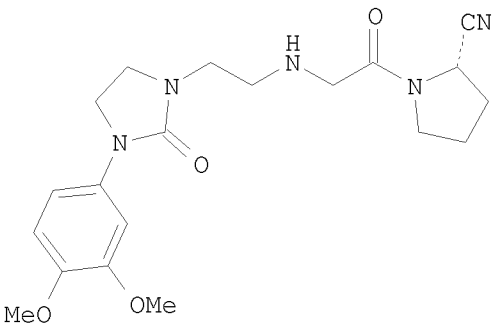


CM 2

CRN 144-62-7
CMF C2 H2 O4



L5 ANSWER 6 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:603998 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 151:148210
TITLE: Synthesis and evaluation of structurally constrained imidazolidin derivatives as potent dipeptidyl peptidase IV inhibitors
AUTHOR(S): Wang, Liutang; Zhang, Bin; Ji, Jianxin; Li, Bogang; Yan, Jufang; Zhang, Weiyu; Wu, Yong; Wang, Xuechao
CORPORATE SOURCE: West China School of Pharmacy, Sichuan University, Chengdu, 610041, Peop. Rep. China
SOURCE: European Journal of Medicinal Chemistry (2009), 44(8), 3318-3322
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Masson SAS
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:148210
GI



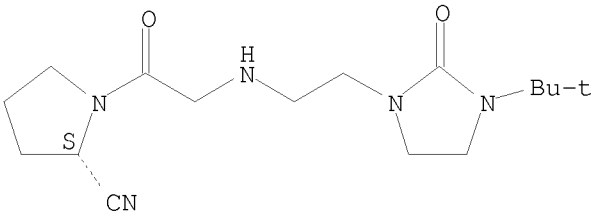
I

AB To find potent and selective inhibitors of dipeptidyl peptidase IV (DPP-IV), a series of 2-cyanopyrrolidine derivs. with constrained imidazolidine ring was synthesized and their activities against DPP-IV were tested. Most of them exhibited submicromolar inhibitory activities against DPP-IV. The most potent compound among these is (S)-1-(2-(2-(3-(3,4-dimethoxyphenyl)-2-oxoimidazolidin-1-yl)ethyl-amino)acetyl)pyrrolidine-2-carbonitrile (I), which is a 2 nM DPP-IV inhibitor.

IT 1145965-57-6P 1145965-60-1P 1145965-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and dipeptidyl peptidase IV inhibitory activity of cyanopyrrolidine derivs. with constrained imidazolidine ring)

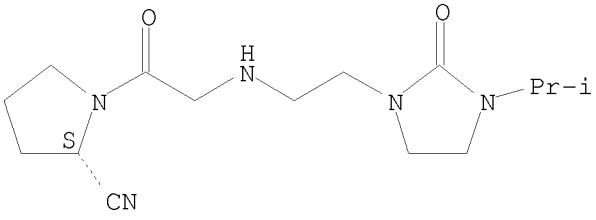
RN 1145965-57-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1,1-dimethylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



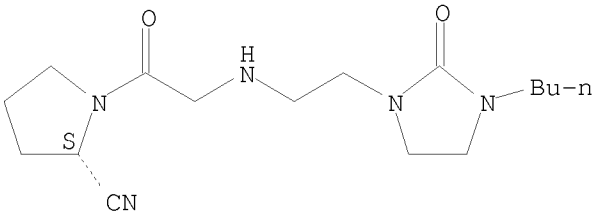
RN 1145965-60-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1-methylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 1145965-65-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-(3-butyl-2-oxo-1-imidazolidinyl)ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

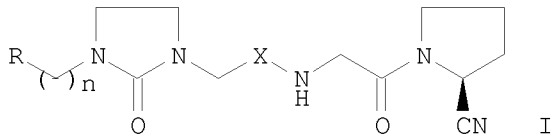


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

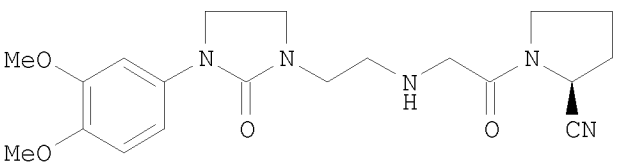
L5 ANSWER 7 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:406944 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 150:448319
TITLE: Preparation of N-substituted pyrrolidine derivatives as DPP-IV inhibitors for treating and/or preventing diabetes mellitus
INVENTOR(S): Wang, Xuechao; Wang, Liutang; Zhang, Bin; Hou, Hui; He, Zhaoquan; Yan, Jufang; Cen, Guodong; Zhang, Weiyu
PATENT ASSIGNEE(S): Chengdu Diao Pharmaceutical Group Co., Ltd., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing, 26pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101397294	A	20090401	CN 2008-10161373	20080923
PRIORITY APPLN. INFO.:			CN 2007-10050091 A	20070924

OTHER SOURCE(S): CASREACT 150:448319; MARPAT 150:448319
GI



I



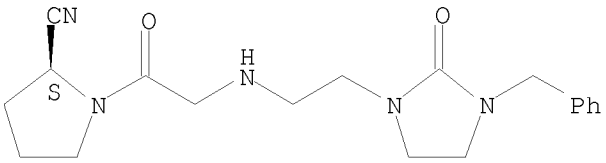
II

AB The title N-substituted pyrrolidine (Gly-Pro dipeptide) derivs. I [wherein n = 0-3; X = CO, CH2, or a bond; R = (un)substituted alkyl, Ph, alkyl, pyridyl, pyridazinyl, pyrazinyl, imidazolyl, pyrazolyl, thiazolyl, etc.] or pharmaceutically acceptable salts thereof were prepared as inhibitors of dipeptidyl peptidase IV (DPP-IV) for treating and/or preventing diabetes mellitus, glucose tolerance disorder, autoimmune diseases, and inflammation. For example, II·oxalate was prepared in a multi-step synthesis. II·oxalate showed inhibitory activity with IC50 of 0.002 μM against DPP-IV. Formulations as tablets and capsules were described.

IT 1145965-56-5P 1145965-57-6P 1145965-60-1P
1145965-65-6P 1145965-70-3P 1145965-71-4P
1145965-78-1P 1145965-82-7P 1145965-86-1P
1145965-92-9P 1145965-96-3P 1145966-03-5P
1145966-04-6P 1145966-06-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of N-substituted pyrrolidine derivs. as DPP-IV inhibitors for treating and/or preventing diabetes mellitus)

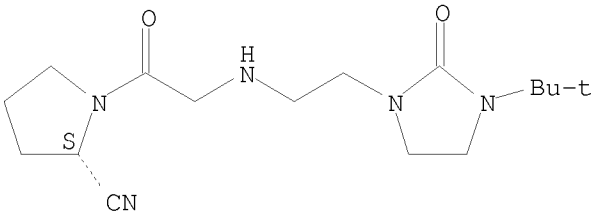
RN 1145965-56-5 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[2-oxo-3-(phenylmethyl)-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 1145965-57-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1,1-dimethylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2008:1210838 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 149:448395
TITLE: 3-Imidazolylindoles for treatment of proliferative diseases and their preparation

INVENTOR(S): Boettcher, Andreas; Buschmann, Nicole; Furet, Pascal; Groell, Jean-Marc; Kallen, Joerg; Hergovich Lisztwan, Joanna; Masuya, Keiichi; Mayr, Lorenz; Vaupel, Andrea
PATENT ASSIGNEE(S): Novartis A.-G., Switz.
SOURCE: PCT Int. Appl., 260pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008119741	A2	20081009	WO 2008-EP53667	20080327
WO 2008119741	A3	20081204		
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
AU 2008234954	A1	20081009	AU 2008-234954	20080327
CA 2682483	A1	20081009	CA 2008-2682483	20080327
AR 65860	A1	20090708	AR 2008-101262	20080327
KR 2009122403	A	20091127	KR 2009-7022526	20080327
EP 2142535	A2	20100113	EP 2008-735532	20080327
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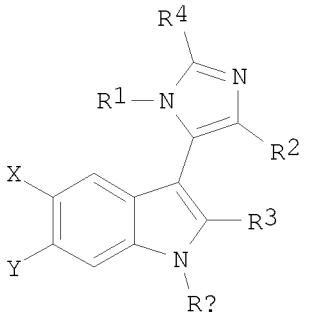
ZA 2009006210	A	20100526	ZA 2009-6210	20090908
CR 11019	A	20091020	CR 2009-11019	20090909
IN 2009DN05959	A	20100611	IN 2009-DN5959	20090916
MX 2009010413	A	20091020	MX 2009-10413	20090928
US 20100125064	A1	20100520	US 2009-593721	20090929
US 8053457	B2	20111108		
CN 101679382	A	20100324	CN 2008-80017611	20091126

PRIORITY APPLN. INFO.: EP 2007-105269 A 20070329
WO 2008-EP53667 W 20080327
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 149:448395; MARPAT 149:448395
GI



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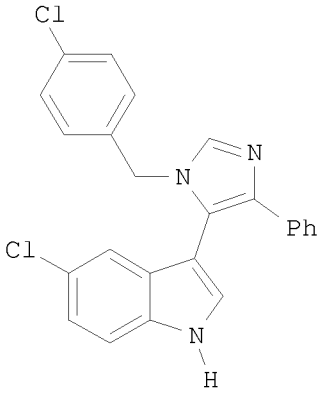


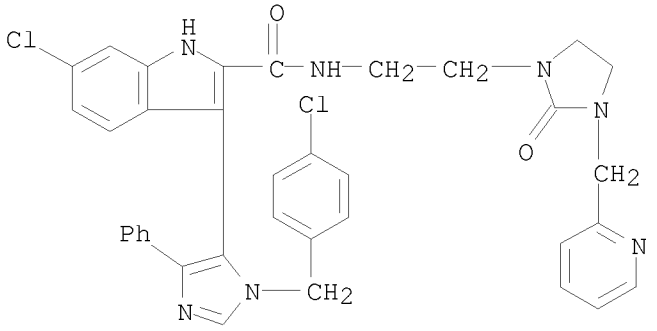
II

AB The invention relates to 3-heterocyclyl indolyl compds. of formula I, which are capable of inhibiting the interaction between p53, or variants thereof, and MDM2 and/or MDM4, or variants thereof, resp. Due to their activity, the compds. are useful in the treatment of various disorders and diseases mediated by the activity of MDM2 and/or MDM4, or variants thereof. Compds. of formula I wherein R1 and R2 are independently (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted aryl and (un)substituted heterocyclyl; R3 is H, halo, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted aryl, carboxy, cyano, etc.; RA is H, (un)substituted alkyl and acyl; X is H, C1-7 (halo)alkyl, C1-7 alkoxy, halo and CN; Y is C1-7 (halo)alkyl, C1-7 alkoxy, halo and CN; and their tautomers, N-oxides and salts thereof, are claimed. Example compound II was prepared by formylation of 6-chloro-1H-indole the resulting 6-chloro-1H-indole-3-carboxaldehyde underwent cyclization with 4-chlorobenzylamine and 1-(isocyanophenylmethanesulfonyl)-4-methylbenzene to give compound II. All the invention compds. were evaluated for their MDM2 and MDM4 inhibitory activity (some data given).

IT 1067657-35-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of imidazolylindoles as MDM2 and MDM4 inhibitors useful in the treatment of proliferative diseases)

RN 1067657-35-5 CAPLUS

CN 1H-Indole-2-carboxamide, 6-chloro-3-[1-[(4-chlorophenyl)methyl]-4-phenyl-1H-imidazol-5-yl]-N-[2-[2-oxo-3-(2-pyridinylmethyl)-1-imidazolidinyl]ethyl]- (CA INDEX NAME)

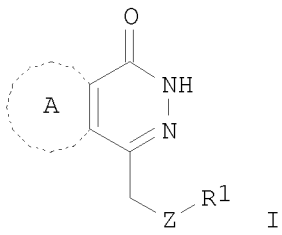


OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)

L5 ANSWER 9 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2008:1157741 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 149:402368
TITLE: Preparation of phthalazinone derivatives for use as PARP inhibitors
INVENTOR(S): Menear, Keith Allan; Hummersone, Marc Geoffrey; Gomez, Sylvie; Javaid, Muhammad Hashim; Martin, Niall Morrison Barr; Kerrigan, Frank
PATENT ASSIGNEE(S): Kudos Pharmaceuticals Limited, UK; Maybridge Limited
SOURCE: PCT Int. Appl., 103pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008114023	A2	20080925	WO 2008-GB990	20080320
WO 2008114023	A3	20081113		
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
US 20080280910	A1	20081113	US 2008-51219	20080319
PRIORITY APPLN. INFO.:			US 2007-896340P P	20070322

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 149:402368; MARPAT 149:402368
GI



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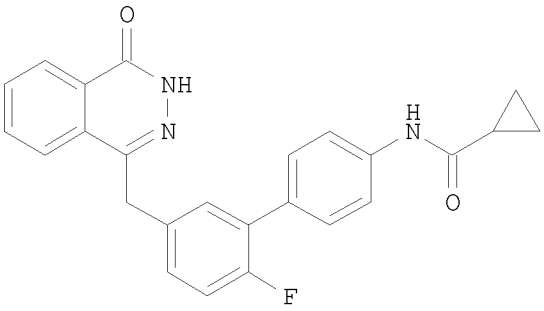


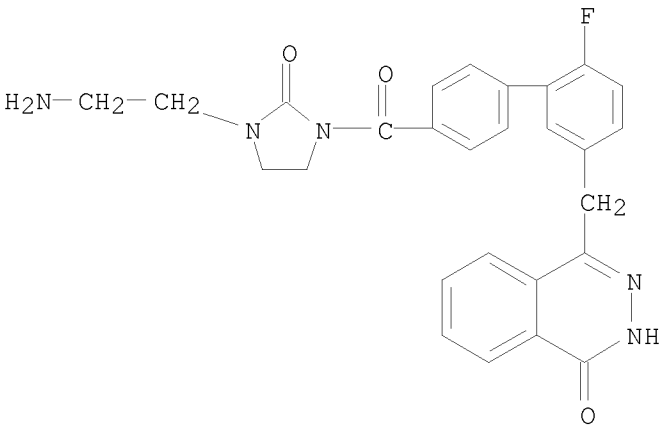
II

AB Title compds. I [Ring A = (un)substituted aromatic or cyclohexene ring; Z = heteroaryl; R1 = (un)substituted aryl bound to Z by a C–C bond; with provisions], and their pharmaceutically acceptable salts, are prepared and disclosed as PARP inhibitors. Thus, e.g., II was prepared by coupling of 4-(3-bromo-4-fluorobenzyl)-2H-phthalazin-1-one (preparation given) with (4-aminophenyl)boronic acid followed by amidation with cyclopropanecarboxylic acid. Select I were evaluated in PARP inhibition assays, e.g., II demonstrated an IC50 value of 0.057 μM.

IT 1062291-39-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalazinone derivs. for use as PARP inhibitors)

RN 1062291-39-7 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[4'-[[3-(2-aminoethyl)-2-oxo-1-imidazolidinyl]carbonyl]-6-fluoro[1,1'-biphenyl]-3-yl]methyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 10 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2007:564518 CAPLUS <<LOGINID::20111214>>
DOCUMENT NUMBER: 147:9799
TITLE: Preparation of piperidine derivatives as antitumor agents
INVENTOR(S): Collibee, Scott; Yang, Zhe; Ashcraft, Luke; Bergnes, Gustave; Morgan, Bradley P.; Morgans, David J., Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 191pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007059323	A2	20070524	WO 2006-US44753	20061115
WO 2007059323	A3	20071227		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
US 20070161674	A1	20070712	US 2006-600684	20061115
US 7572814	B2	20090811		
AR 58839	A1	20080227	AR 2006-105001	20061115
EP 1962846	A2	20080903	EP 2006-837964	20061115
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				

PRIORITY APPLN. INFO.: US 2005-737226P P 20051115
WO 2006-US44753 W 20061115
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 147:9799; MARPAT 147:9799
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Piperidine derivs. I, wherein X is chosen from =O and =N-OR, where R is selected from hydrogen and alkyl, provided that at least one =X is =O, R1 is chosen from hydrogen, alkyl, cycloalkyl, heterocycloalkyl, aryl and heteroaryl; R2 is chosen from aryl, heterocycloalkyl, alkyl, cycloalkyl, heteroaryl, alkoxy, hydroxy, and amino; R3 is chosen from hydrogen and alkyl; R4 is chosen from hydrogen, alkyl, heterocycloalkyl, acyl, aryl, heteroaryl, amino-carbonyl, sulfonyl, alkoxycarbonyl, and cycloalkyl; R5 is chosen from hydrogen and alkyl; and R6 is chosen from aryl,

heterocycloalkyl, alkyl, cycloalkyl, heteroaryl, alkoxy, hydroxy, and amino, were prepared via cyclocondensation of methylene derivs. with primary amines, and used for treating cellular proliferative diseases. Thus, cyclocondensation of methylene II with benzylamine gave piperidine III, which was used as intermediate in synthesis of title compds. Thus, (cis,trans)-1-(2-hydroxyethyl)-4-phenyl-5-(phenyl-carbonyl)(3-piperidyl)phenyl-ketone was prepared and tested in vitro and in nude mice as antitumor agent. In vitro potency of chemical entities provided herein can be determined, for example, by assaying human ovarian cancer cells (SKOV3) for viability following a 72-h exposure to a 9-point dilution series of compound The composition of title compds. is formulated in a form chosen from injectable fluids, aerosols, creams, gels, tablets, pills, capsules, syrup; ophthalmic solns., and patches. Certain of the chemical entities described herein were evaluated for in vivo activity against SKOV-3 human ovarian carcinoma in a tumor growth delay (TGD) study. The study utilized eight groups (n = 8) of athymic nude mice bearing established (63-144 mm3) SKOV-3 tumors on day 1, and included a vehicle-treated tumor growth control group and a reference group treated with paclitaxel (30 mg/kg i.v. qod x 5). Title compds. were evaluated at doses of 300 or 150 mg/kg administered i.p. once daily and at 150 mg/kg administered i.p. twice daily. The 250 and 500 mg/kg once daily treatments produced 15 and 58 % TGD, resp., which was statistically significant activity at 500 mg/kg. The 250 mg/kg twice daily treatment produced 57 % TGD, which was statistically significant activity.

IT 937713-50-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidine derivs. as antitumor agents via cyclocondensation of methylene derivs. with primary amines)

RN 937713-50-3 CAPLUS

CN 2-Imidazolidinone, 1-[2-(dimethylamino)ethyl]-3-[2-[(3R,5S)-4-(3-fluoro-2-methylphenyl)-3,5-bis(3-hydroxybenzoyl)-1-piperidinyl]ethyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.